3,4-Pyridinediamine, 5-nitro-

Other names: 3,4-Diamino-5-nitropyridine
Inchi: InChI=1S/C5H6N4O2/c6-3-1-8-2-4(5(3)7)9(10)11/h1-2H,6H2,(H2,7,8)
InchiKey: OMUADEPNIQXNRG-UHFFFAOYSA-N
Formula: C5H6N4O2
SMILES: Nc1cncc([N+](=O)[O-])c1N
Mol. weight [g/mol]: 154.13
CAS: 4318-68-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.16		Crippen Method
logp	0.154		Crippen Method
mcvol	104.910	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4318687&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume